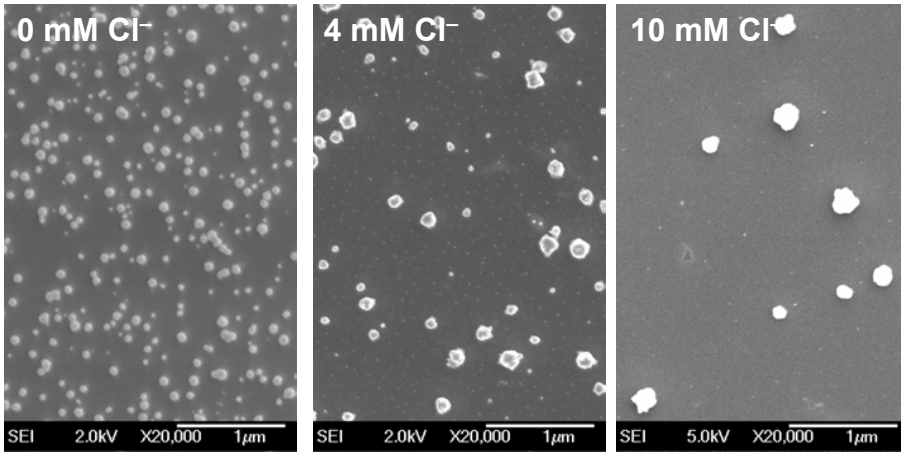
Fundamental Aspects of Electrocrystallization: an Experimental and Modeling Approach

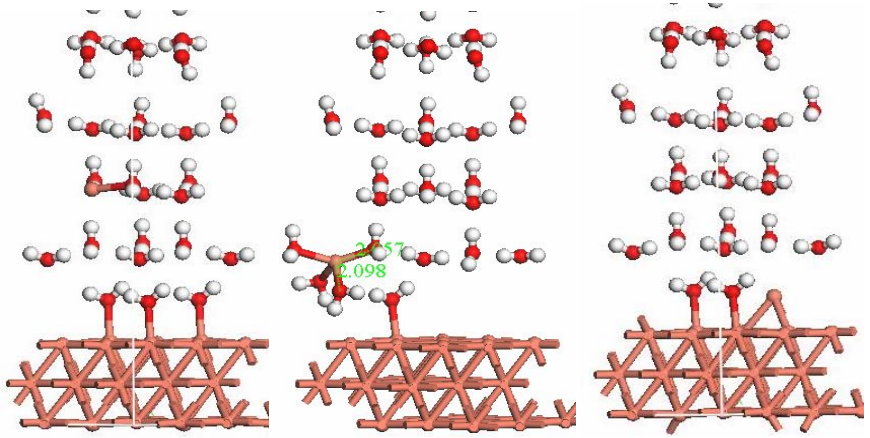
Giovanni Zangari, University of Virginia – DMR-0093154

Fundamental understanding of metal growth from electrolytic solutions is pursued through coupled experimental and modeling efforts.

In the instance shown here, we are attempting to understand some features of the growth process (here, the decrease in nucleation density of Cu on Si by addition of chlorides) by simulating the electrodeposition process at the atomic scale to extract fundamental parameters (in this case, the nucleation probability) for the phenomenon of interest.



Morphology of copper nuclei grown on Si(100) from a sulfate electrolyte with varying additions of Cl–.



Configuration of the electrolyte/Cu interface determined by a density functional theory method, showing the discharge process of a Cu ion initially in solution

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Education:

Three graduate students (G. Ofori-Boadu, W. Shao, X. Xu) and one post-doc (G. Pattanaik) are contributing to this work.

A graduate course on applied electrochemistry and electrodeposition of metals will be broadcasted through the Commonwealth of Virginia in the framework of the CGEP program at UVa.

Lectures on "How to make materials with electrochemistry" have been offered in the framework of an undergraduate course at U. Virginia on "Materials that shape civilization"

Broad Impact:

Several invited talks at conferences in Europe and the US have been delivered during 2004

Outreach:

Various demonstration on the impact of electrochemistry in our daily lives – from corrosion to the production of components for cell phones, cars and computers have been offered to high school and visiting undergraduate students.

Gyana Pattanaik with students at the 2003 UVA Materials Science Majors Open House.